Advanced Simulation Capability for Environmental Management (ASCEM)

The Multi-Process HPC Simulator

September 1, 2010.

1. Background
   - Bridging Communities in this new Community Code
2. Multi-Process HPC Simulator
   - Tasks Under the HPC Simulator
3. FY11 and Beyond

Outline

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Motivation and High Level Objectives of ASCEM

The objective of ASCEM is to develop a state of the art scientific tool and framework for understanding and predicting contaminant fate and transport in natural and engineered systems. The modular and open source high performance computing tool will facilitate integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for EM cleanup and closure activities.

ASCEM will build upon national capabilities developed from decades of research and development in subsurface geosciences, modeling and simulation, and environmental remediation. In addition, the integrated toolset will incorporate capabilities for predicting releases from various waste forms, identifying exposure pathways, performing dose calculations, and conducting systematic uncertainty quantification.

Developing a Broader Sense of Community

There have been significant advances in numerical methods over the last 10-15 years, and many of these advances have not made there way into production flow and reactive transport simulation codes.

There have been significant advances in software engineering, high-level and object-oriented languages, and algorithmic abstractions over the last 10-15 years, and many of these advances have not made there way into production flow and reactive transport simulation codes.

There is significant expertise in the geosciences community related to subsurface multi-phase flow and reactive-transport applications, including mathematical models, formulations, and numerical methods.

ASCEM strives to establish a new community that bridges these distinct groups, truly building on the best from each.

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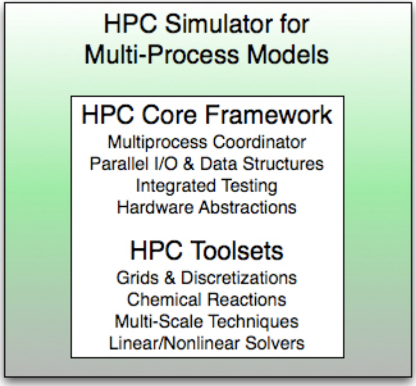
Multi-Process HPC Simulator Tasks



Approach

1. **Process Models** implemented at high level and driven by the platform toolsets.
2. **HPC Core Framework** provides necessary low-level services.
3. **HPC Toolsets** provide flexible access to advanced numerical methods and solvers.

Process Models

Provide mathematical description of the processes that play a role in the release and transport of contaminants in the environment.

- Define the mathematical formulation of process models for
  - Single/multiphase flow and infiltration processes,
  - multicomponent transport processes,
  - chemical and biological processes,
  - complex source terms (e.g., cementitious barriers).
- Evaluate model properties that impact HPC simulator, such as time scales of relevant coupled processes and heterogeneity.
- Prioritize process models and their coupling, based on relevant applications and site data.
- Develop objects and interface designs for flexible, high level representation models accessible to domain scientists.

HPC Core Framework

Provide key infrastructure to facilitate modular design of the HPC simulator, portability and a graded quality assurance approach.

- Provide low-level services, such as
  - Parallel input/output and parallel (distributed) data structures
  - Guide API design and provide HPC related visualization support
  - Leverage elements of existing frameworks such as Trilinos and PETSc
- Implement unified hierarchical approach to testing, verification and validation, and benchmarking (integrated tests)
- Use automated, cross-platform builds to ensure robust and efficient performance on a range of platforms from laptops to supercomputers

HPC Toolsets

Provide the building blocks that transform the mathematical description of the process models into a discrete form suitable for computer simulation.

- Provide Multiprocess Coordinator (MPC) services that coordinate the assembly of coupled-process simulations from the HPC Toolsets
- Distributed parallel mesh data structures that serve to bridge the conceptual model and the numerical methods (Meshing Toolset)
- Fundamental building blocks to create the process models (Discretization Toolset)
- Algorithms to solve the discrete nonlinear systems of equations that arise in EM applications (Solvers Toolset)

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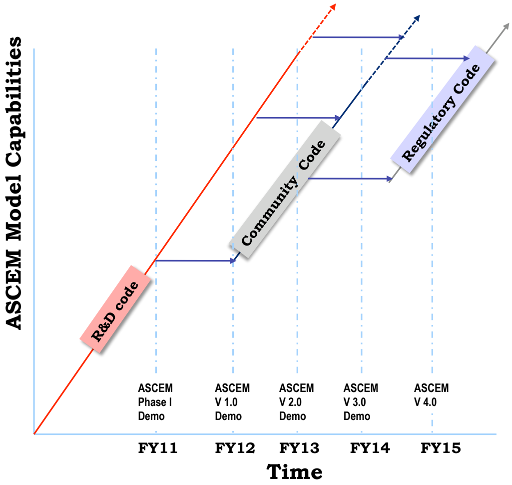
A Canonical ASCEM Year

1. internal review of last years development and demonstration
2. develop this years demonstration targets
3. external review of code status, demonstration, and plans
4. revisit and update requirements and design documents
5. prototype and then release the next version of the code
6. perform and report on the demonstration

Release Branches and Proposed Schedule



Tentative Process Model Targets

1. weakly coupled modeling of flow, transport and reaction (2010)
2. options for more strongly coupled simulation (2011)
3. high-ionic strength geochemistry (starting 2011?)
4. intrusive forward and adjoint sensitivity
5. weak moving to strong coupling with CBP (starting 2011)
6. multi-phase multi-component flow?
7. fractured media and multiscale techniques, potentially including particle tracking methods (starting 2012)
8. non-isothermal processes and geo-mechanical (linear elasticity)
   - weak coupling (operator splitting) in 2013
   - strong/tight coupling in 2014
9. CO_2 specific and relevant processes (help us prioritize)